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Colloquia: Channeling 2010

Modeling of thermal neutrons channeling in nanotubes with surface circular currents

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Summary. — The numerical simulation of thermal neutron channeling in conical and curved nanotubes with large circular surface currents is carried out. The coordinate distribution of neutrons from the impact parameters and the surface current density is obtained. It is demonstrated that thermal neutrons can be focused after they have left the tube end. The condition for the retention of a neutron along the curved nanotube is obtained. The dependence of the surface current J on the neutron velocity V is found to be described by the correlation $J = 1.465 \times 10^{-5}$ V.

PACS 61.85.+p – Channeling phenomena (blocking, energy loss, etc.).

1. – Introduction

Neutron polycapillary optics was first suggested by M. A. Kumakhov about 25 years ago. Polycapillary technologies enable creation of neutron diffractometers, spectrometers, reflectometers, microscopes—all with a micrometer-size focal spot [1,2]. New instruments of neutron optics are portable and highly efficient [2]. So, neutron polycapillary optics makes it possible to create new instruments for scientific research, and allows the neutron beams to be used for industrial applications [1-3].

The comprehensive review and theoretical consideration of channeling of neutral particles like photons and neutrons in carbon nanotubes can be found in the work [4]. Usually the phenomenon of channeling takes place due to coherent scattering of the neutrons on the crystal planes or on the capillaries walls. But in some cases other mechanisms might be of vital importance. As was shown by V. I. Tsebro *et al.* [5,6], carbon nanotubes can be very efficient conductors, in their characteristics comparable with superconductors. Namely, a closed system of carbon nanotubes twining round a tube with a diameter of approximately 50 nm can support electrical current for 15 hours at room temperature. Further it was demonstrated [7] that the current-carrying capacity and reliability studies of multiwalled carbon nanotubes under high current densities ($> 10^9$ A/cm^2) show

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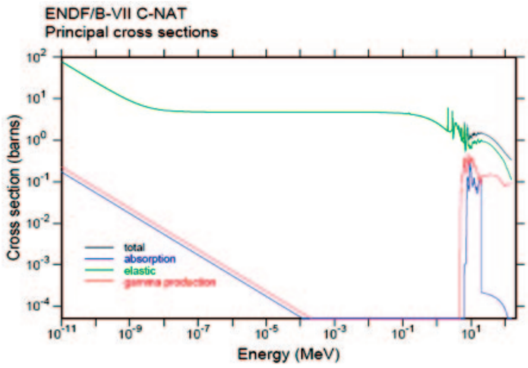

Fig. 1. – Energy dependence of neutron interaction in carbon [8].

that no observable failure in the nanotube structure and no measurable change in the resistance were detected at temperatures up to 250 °C and for time scales up to 2 weeks. For such currents the magnetic field inside the carbon nanotube reaches up to 10^{10} G that could be meaningful for neutrons channeling along the tube. Accordingly, one can use the magnetic fields generated by such currents to control the neutron beams, for example, in neutron capture therapy.

2. – Basic mechanisms of neutrons interaction with a nanotube

The range of neutron energies considered in this paper is 0.025–1 eV. Corresponding to this energy range the neutron velocity is equal to 2–14 km/c. As can be seen from fig. 1 in this energy range the cross-section of their elastic interaction of neutrons with the carbon atom is significantly higher than other cross-sections.

Let us consider neutron scattering on the nanotube surface in the Born approximation. In this approach the particle states can be described by plane waves, incident and reflected, respectively:

$$|\mathbf{k}\rangle = \exp[i\mathbf{kx}], \qquad |\mathbf{k}'\rangle = \exp[i\mathbf{k}'x]. \tag{1}$$

The Hamiltonian of interaction is defined as

$$H = \Sigma V(\mathbf{x} - \mathbf{x}_j), \quad j = 1, 2, \ldots, N, \tag{2}$$

where $\mathbf{x}_j$ is the radius vector of the atom with number j; N is the number of atoms in the nanotube. As known the scattering is described by the matrix elements

$$\langle \mathbf{k}'m|\mathbf{H}|n\mathbf{k}\rangle = \left\langle m \left| \int \mathrm{d}^3\mathbf{x} e^{i(k-k')x} \mathbf{H} \right| n \right\rangle = V_k \sum \left\langle m|e^{i(k-k')x}|n \right\rangle, \tag{3}$$

where

$$V_k = \int \mathrm{d}^3\mathbf{x} e^{i(k-k')x} V(\mathbf{x}). \tag{4}$$

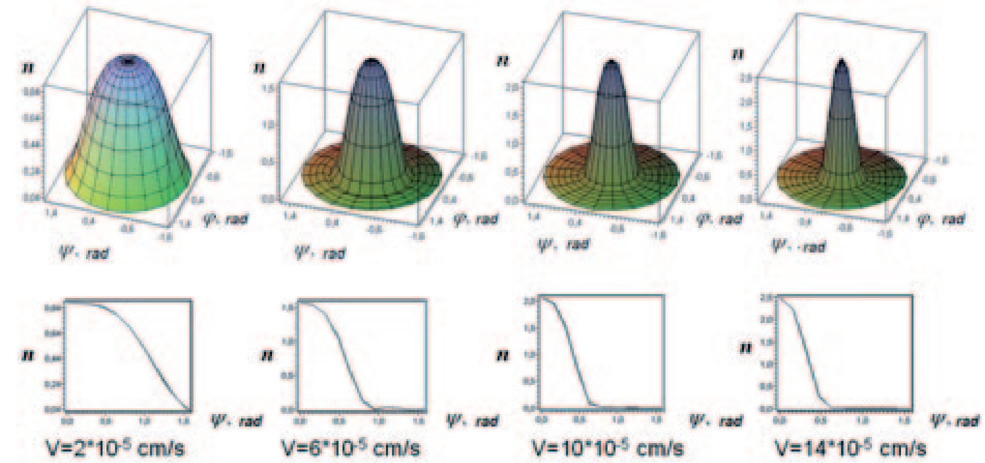

Fig. 2. – Probability density of the angular distribution of neutrons for different neutron velocities v.

The elastic coherent scattering of neutrons by a chain of atomic nuclei can be described by a small repulsive potential $U \leq 2\text{–}3 \times 10^{-7}\,\text{eV}$ acting on the neutrons. Therefore, neutrons with energy $\varepsilon = 0.025\,\text{eV}$ hitting the surface at an angle $\alpha \leq \sqrt{(U/\varepsilon_0)} \approx 10^{-3}\,\text{rad}$ (the Lindhard angle) are mainly reflected. So, the elastic scattering cannot influence the neutron trajectory at grazing incidence angles larger than $10^{-3}\,\text{rad}$.

Without describing the method in details, below we present the results of numerical simulations for the particle angular distributions (fig. 2). From it one can see that the elastic scattering cannot change essentially the neutron trajectory. Indeed, the graphs for different speeds of neutrons are symmetric with respect to zero position. That can be explained by the fact that the considered nanotube wall thickness is of one atomic layer, and, hence, such a wall is fairly transparent for neutrons.

Now we move our consideration to another mechanism of neutrons interaction with matter, *i.e.* the interaction between the neutron magnetic moment and the magnetic field of surface currents.

3. – Channeling in a conical nanotube

At distances much larger than the interatomic distance in a nanotube one can apply a classical approach to study the neutron penetration. Following the works [1-3], carbon nanotubes can accept a huge current density of the order of $1.8 \times 10^{10}\,\text{A/cm}$, and keep them for a long time. Therefore, we consider the interaction of the magnetic field produced by these currents with the magnetic moment of neutrons. This field can be derived from the Biot-Savart law:

$$\mathbf{H} = \frac{1}{c} \int \frac{[\mathbf{j}, \mathbf{R}]}{R^3} \mathrm{d}V. \tag{5}$$

The interaction potential then is defined as $U = \mu\mathbf{H}$.

Let us consider the passage of neutrons through a conical nanotube of various ratios between input and output nanotube radii (see fig. 3). The field inside the nanotube

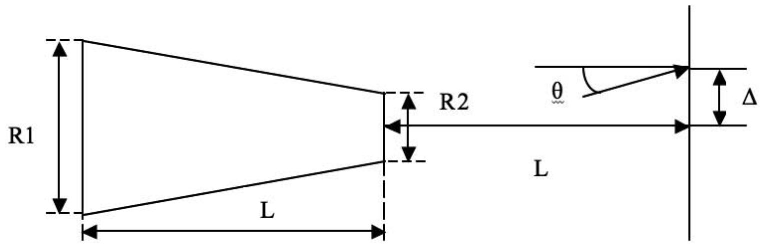

Fig. 3. – The scheme of neutron passage through a conical nanotube.

(fig. 4) is given by the formulas:

$$
(6)\quad
\begin{aligned}
H_r &= \frac{J}{c}\int_0^L\int_0^{2\pi}\frac{(z_0-z)\sin\phi}{\sqrt{((R(z)\cos\phi)^2+(r_0-R(z)\sin\phi)^2+(z_0-z)^2)^3}}\,\mathrm{d}\phi\,\mathrm{d}z,\\
H_z &= \frac{J}{c}\int_0^L\int_0^{\pi}\frac{r_0\sin\phi-R(z)}{\sqrt{((R(z)\cos\phi)^2+(r_0-R(z)\sin\phi)^2+(z_0-z)^2)^3}}\,\mathrm{d}\phi\,\mathrm{d}z.
\end{aligned}
$$

Here $R(z) = R_1 - (R_1 - R_2)/L_z$, where R_1 , R_2 are the nanotube ends radii, r_0 , z_0 are the parameters of the input neutron beam, L is the nanotube length. It is supposed that the ring currents of density J flow on the surface of a nanotube. A beam of thermal or epithermal neutrons hits the end of the nanotube: the beam is homogeneous and parallel to the z-axis. Our purpose is to calculate numerically the current density J that allows neutrons channeling for energies from thermal to epithermal. Also, we obtain the distribution of neutrons at the nanotube end.

The neutrons distribution can be numerically calculated using the above given formulas. We calculate the neutrons distribution at the exit distances equal to the nanotube length. Also, we define: $\Delta(\rho,\, J)$ as the distance from the axis of nanotube to the point of hitting the target, and the $\theta(\rho,\, J)$ as the incidence angles corresponding to these R_{otar} where ρ is the impact parameter. The simulation result is given in figs. 5, 6.

For these graphs (figs. 5 and 6) we can determine the characteristics of nanotube that will be optimal for the neutron beam focusing. All graphs on figs. 5, 6 in projection converge almost at one point on the left. This is because of the fact that the closer to the center of the nanotube, the smallest the magnetic field gradient, which leads to neutrons deviations as compared to the initial impact parameter. On the contrary, far from the

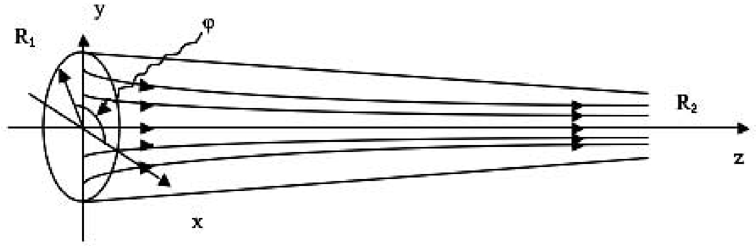

Fig. 4. – Magnetic field inside the nanotube.

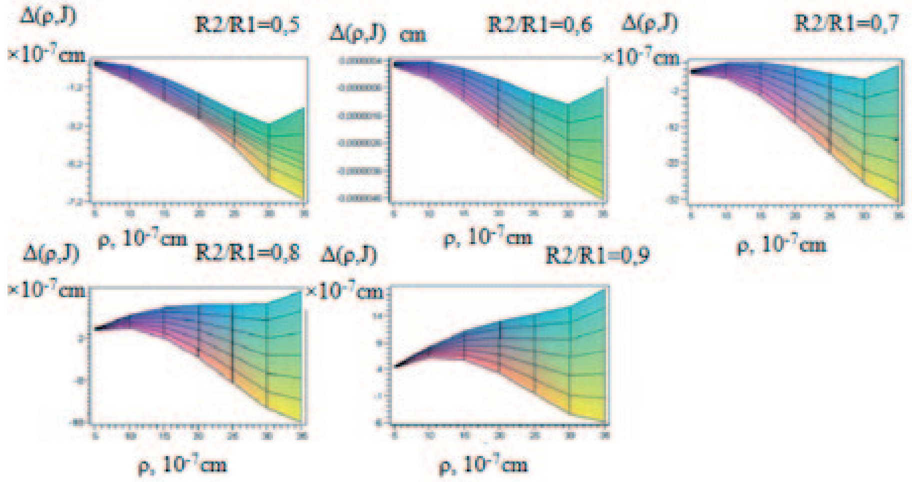

Fig. 5. – Spatial distribution of neutrons.

center of the nanotube the magnetic field gradient is not monotonically increasing to the edge, which is demonstrated by the trajectories self-intersection for neutrons with different impact parameters on some of the graphs. Therefore, to obtain the minimum focal spot at a greater R_2/R_1 relation it is necessary to increase the surface current density. Also from figs. 5, 6 one can see that the minimum diameter of the focal spot is obtained when the ratio is $R_2/R_1 = 0.7$. Figures 7 and 8 present the three-dimensional angular and spatial distributions of the minimum focal spot.

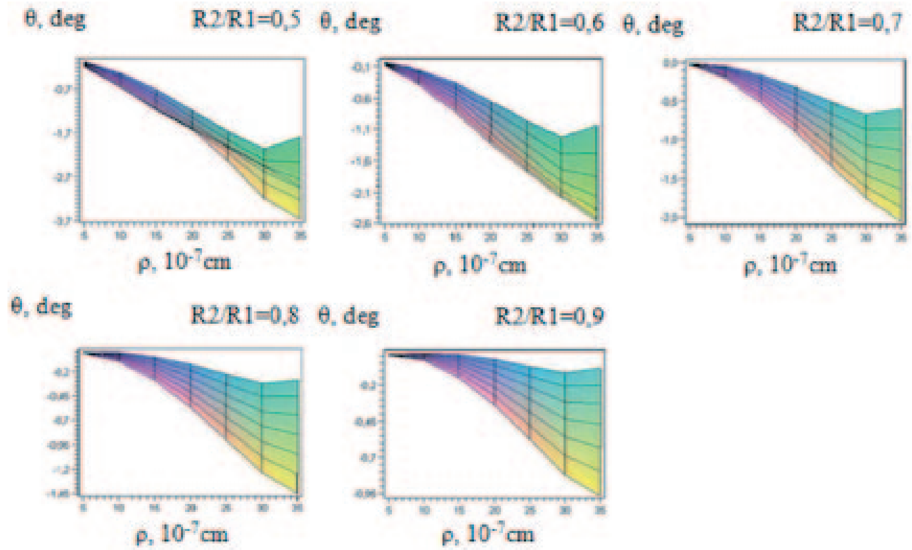

Fig. 6. – Angular distributions of neutrons.

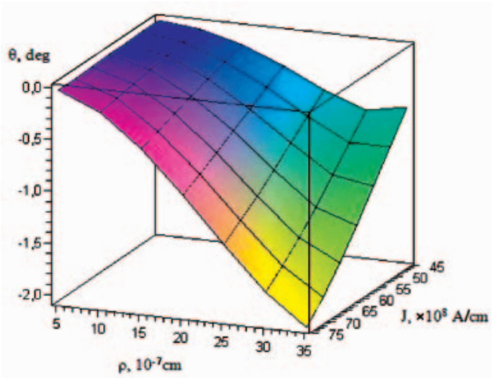

Fig. 7. – Angular distribution of neutrons, at a distance about the length of the nanotube from its end, *versus* the current density J and impact parameter ρ.

4. – Channeling in a curved nanotube

Let us consider a nanotube with radius r and radius of curvature R. For the nanotube with dimensions $r = 50 \times 10^{-7}$ cm, $R = 500 \times 10^{-7}$ cm and for different neutron velocities V one can calculate the surface current density J. For this we consider only the neutrons in the condition when the neutron is strictly fixed at the axis of nanotube. For such J it is possible to calculate the ratio $\delta = d_e/d_o$, which is the ratio of the entrance neutron beam diameter to the output diameter. The beam diameter at the entrance was taken $d_e = 3 \times 10^{-7}$ cm. Below we give the results of numerical simulations for it.

The neutrons trajectories in a bent nanotube are represented in fig. 9. The results of neutron scattering for the other velocities V do not drastically differ from what above stated.

In order to determine the dependence of J on V, it was build a graph (see fig. 10) of the logarithmic dependence of J on V for the relevant data given in table I using the method of the least squares. The slope coefficient is defined by the relation $J = 1.465 \times 10^{-5}\,\mathrm{V}^2$.

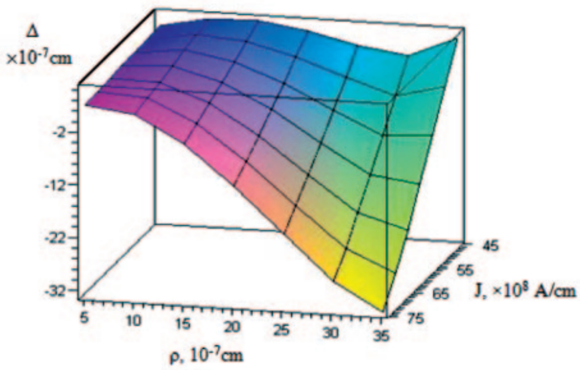

Fig. 8. – Spatial distribution of neutrons, at a distance about the length of the nanotube from its end, *versus* the current density J and impact parameter ρ.

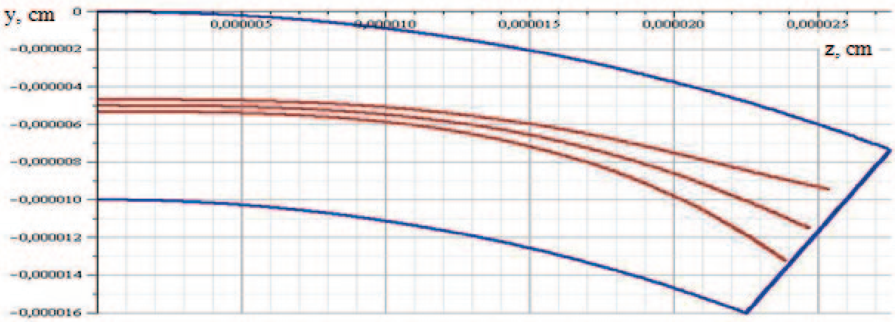

Fig. 9. – Trajectory of the neutron with velocity $V = 200000\,\mathrm{cm/s}$ in a bent nanotube.

Here it is should be underlined that at small impact parameter the neutron deviations from the center lead to more rejection. This means that a curved nanotube with strong surface currents can be used to manufacture a high-precision neutron spectrometer, as well as to control the narrow thermal neutron beams with a certain energy, for example, for medical or other applications.

5. – Conclusion

The possibility of neutron beam focusing and control using carbon nanotubes was investigated in this work. Neutrons with energies 0.025–1 eV are considered. At these energies neutrons have a speed of the order of 2–14 km/s. The cross-sections of the elastic scattering of such neutrons on carbon atoms are significantly higher than inelastic ones, thus, we can consider only the elastic scattering on the nanotube wall. On the other hand, the elastic scattering in this case cannot change the neutron trajectory considerably because the nanotube wall is considered to be very thin and transparent

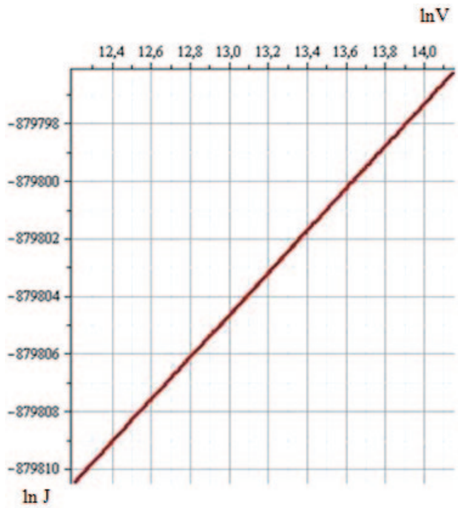

Fig. 10. – Graph of the logarithmic dependence of J as a function of V.

TABLE I. – *The dependence of current density J and ratio δ of the entrance neutron beam diameter to the output diameter on the velocity of neutrons V.*

V (cm/c)	J (A/cm)	δ
200000	586700	6.5994
300000	1320000	6.5994
400000	2347000	6.5995
500000	3667000	6.5995
600000	5281000	6.5996
700000	7188000	6.5996
800000	9389000	6.5996
900000	11883000	6.5996
1000000	14671000	6.5997
1100000	17751000	6.5997
1200000	21127000	6.5997
1300000	24795000	6.5997
1400000	28754000	6.5997

for thermal neutrons. However, due to strong surface currents another mechanism of neutrons interaction with matter may take place: the interaction between the magnetic moment of the neutron and the magnetic field. As shown by Tsebro *et al.* [5,6], nanotubes allow a large current density to pass through and in addition they are able to maintain the induced current during a few hours at room temperature. In this respect, later results by Wei *et al.* [7] demonstrate even a stronger effect. Based on this and assuming that on the nanotube surface the surface current exists, the neutrons passage through conical and curved nanotubes has been numerically simulated. The optimal characteristics of the nanotube that would be best from the point of view of the neutron beam focusing were determined. The neutrons passage through a curved nanotube was considered. In this case our aim was to find the condition for the neutron retention in the center of the channel. As a result of numerical modeling the $J = f(V)$ dependence was evaluated. We suppose that the results obtained may be of use for controlling the narrow thermal neutron beams with a certain energy, for example, for medicine applications in neutron capture therapy.

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